



## Investigation of NO<sub>x</sub> and CO Formation at Ultra-Wet Conditions

**Göke, Sebastian; Schimek, Sebastian; Fateev, Alexander; Clausen, Sønnik; Kuhn, Phoebe; Terhaar, Steffen; Paschereit, Christian Oliver**

*Publication date:*  
2011

[Link back to DTU Orbit](#)

### *Citation (APA):*

Göke, S. (Author), Schimek, S. (Author), Fateev, A. (Author), Clausen, S. (Author), Kuhn, P. (Author), Terhaar, S. (Author), & Paschereit, C. O. (Author). (2011). Investigation of NO<sub>x</sub> and CO Formation at Ultra-Wet Conditions. Sound/Visual production (digital)

---

### General rights

Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

# Investigation of NO<sub>x</sub> and CO Formation at Ultra-Wet Conditions

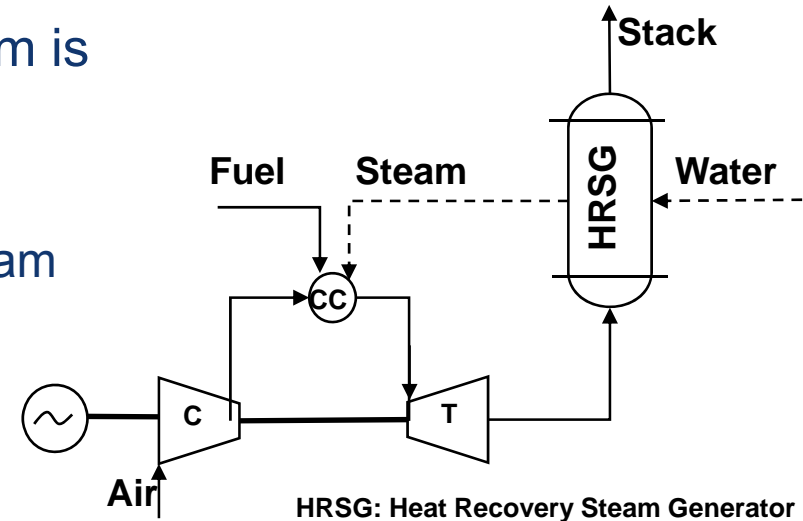
Sebastian Göke, Sebastian Schimek, Alexander Fateev, Sonnik Clausen,  
Phoebe Kuhn, Steffen Terhaar, Christian Oliver Paschereit

Chair of Fluid Dynamics  
- Hermann Föttinger Institute –  
Technische Universität Berlin



The research leading to these results has received funding from the European Research Council under the ERC grant agreement no 247322, GREENEST.

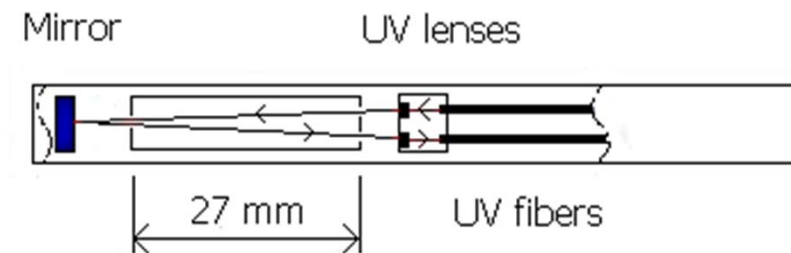
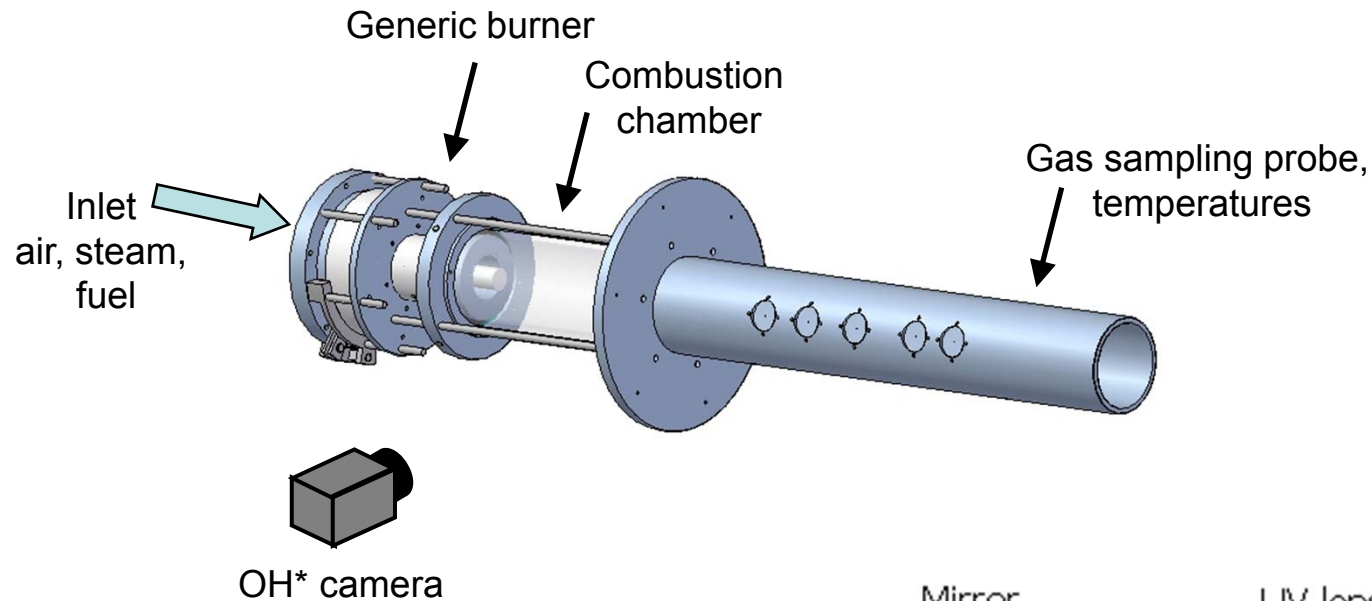
- In humid gas turbines, water or steam is injected into the cycle
- Efficiency increase:
  - Use of exhaust heat to generate steam
  - Improved cooling
- Reduced  $\text{NO}_x$  emissions:
  - Lower flame temperature
  - Influence on chemical reactions
- Clean combustion of syngas and hydrogen



- Combustion at ultra-wet conditions allows for
  - Further increased efficiency up to 55-60% in single cycle application
  - $\text{CO}_2$ -sequestration: near-stoichiometric combustion leads to high concentration of  $\text{CO}_2$  after condensation of the steam

- Initial assessment of atmospheric combustion at ultra-wet conditions
- Development of a modeling tool for reaction kinetics
- Influence of steam on
  - Flame shape
  - Combustion process
  - Emissions formation

- Motivation and Background
- **Experimental Setup and Results**
- Design of Reactor Network and Validation
- Results of Network Model
- Conclusions

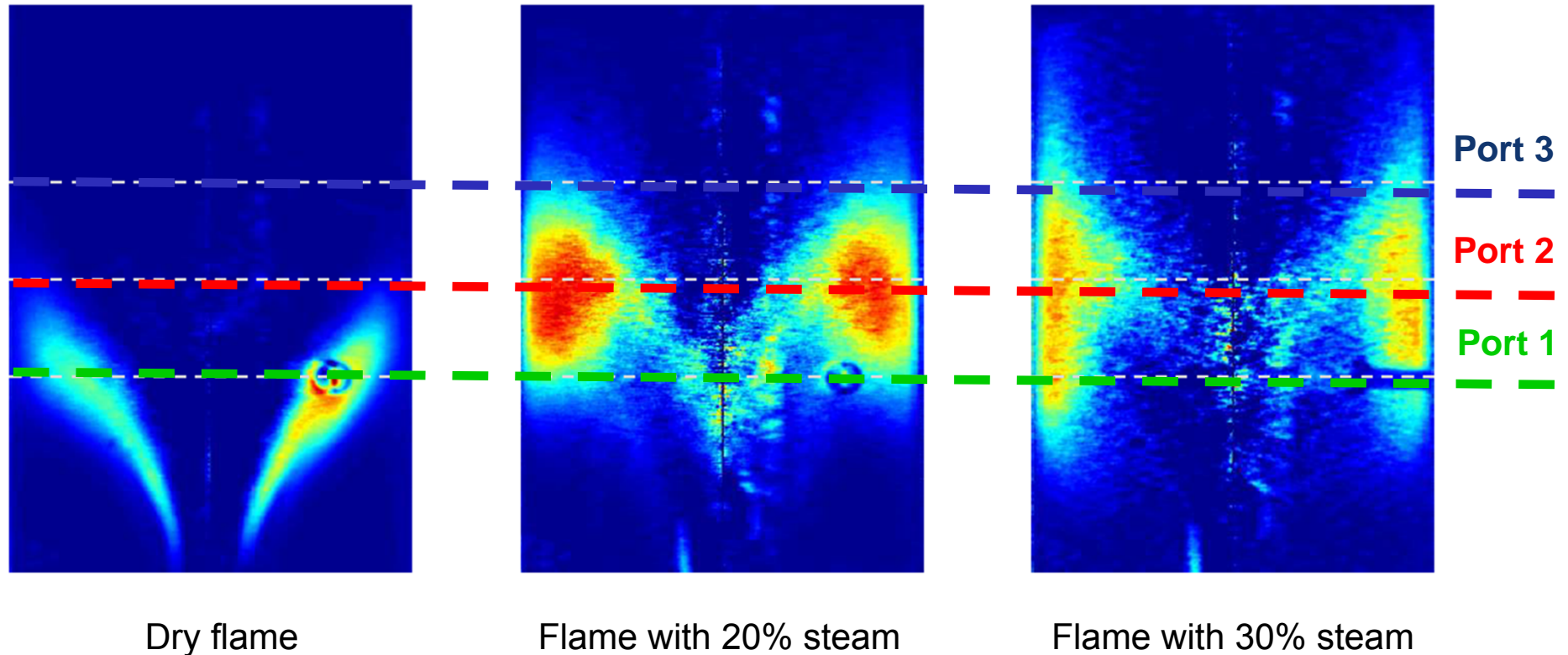


### Operating conditions:

- Inlet temperature: 200°C and 370°C
- Degree of humidity:
  - $\Omega = \dot{m}_{\text{steam}} / \dot{m}_{\text{air}}$
  - $\Omega = 0\% - 30\%$

# OH\* Chemiluminescence:

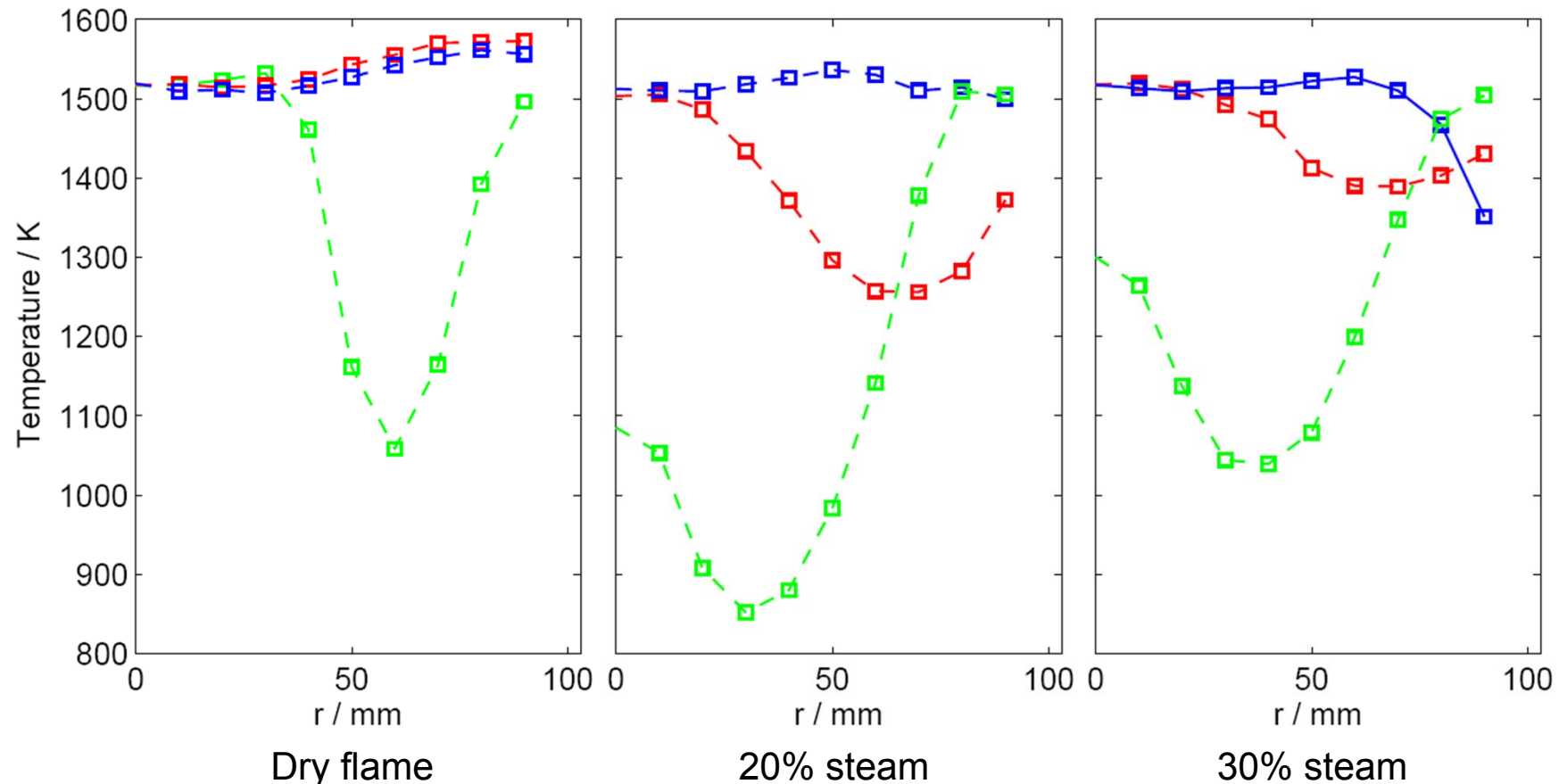
Steam increases region of heat release



$$T_{ad} = 1850 \text{ K}$$

# Flame Temperature:

Flame not significantly longer

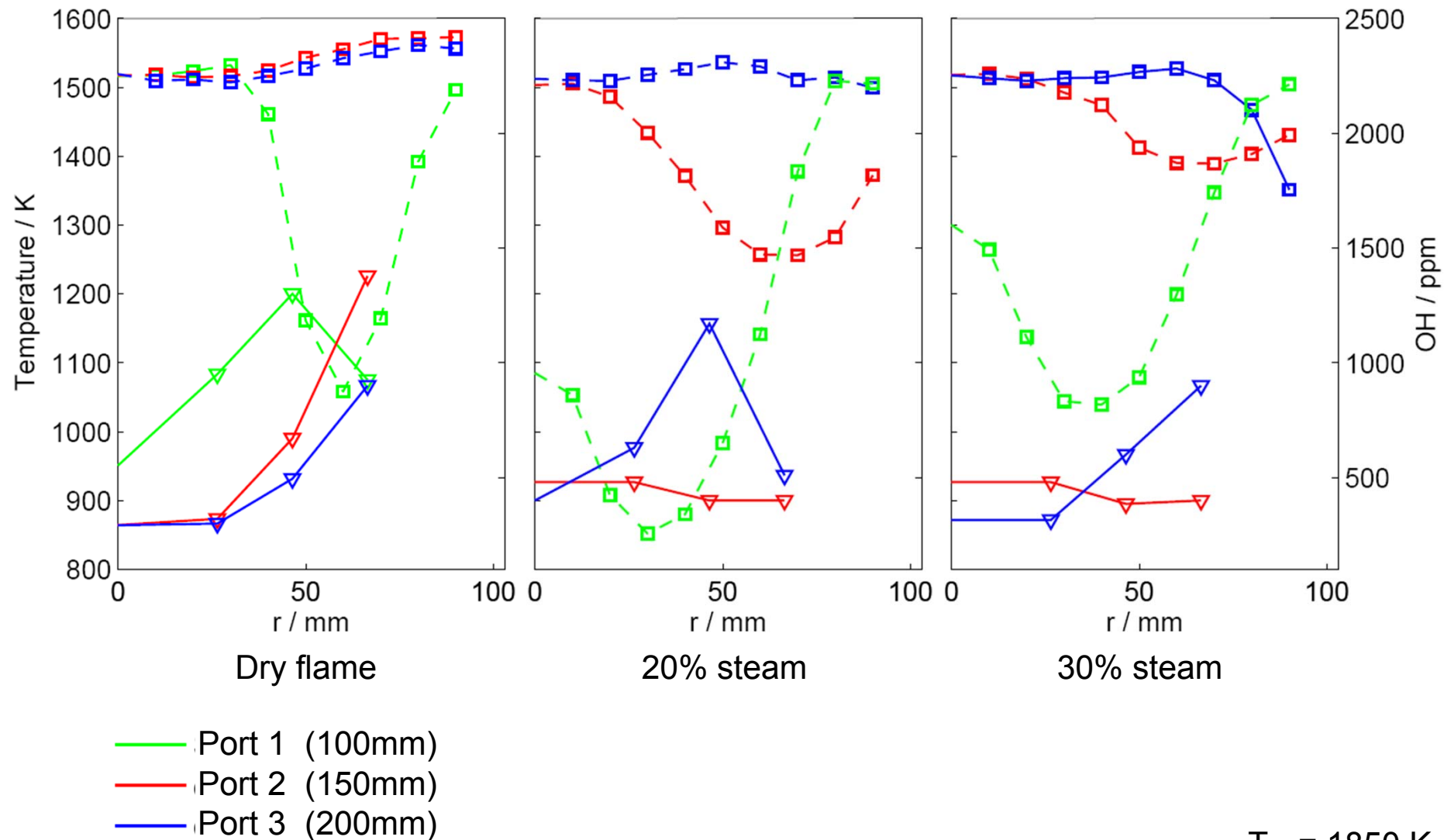


- Port 1 (100mm)
- Port 2 (150mm)
- Port 3 (200mm)

$$T_{ad} = 1850 \text{ K}$$



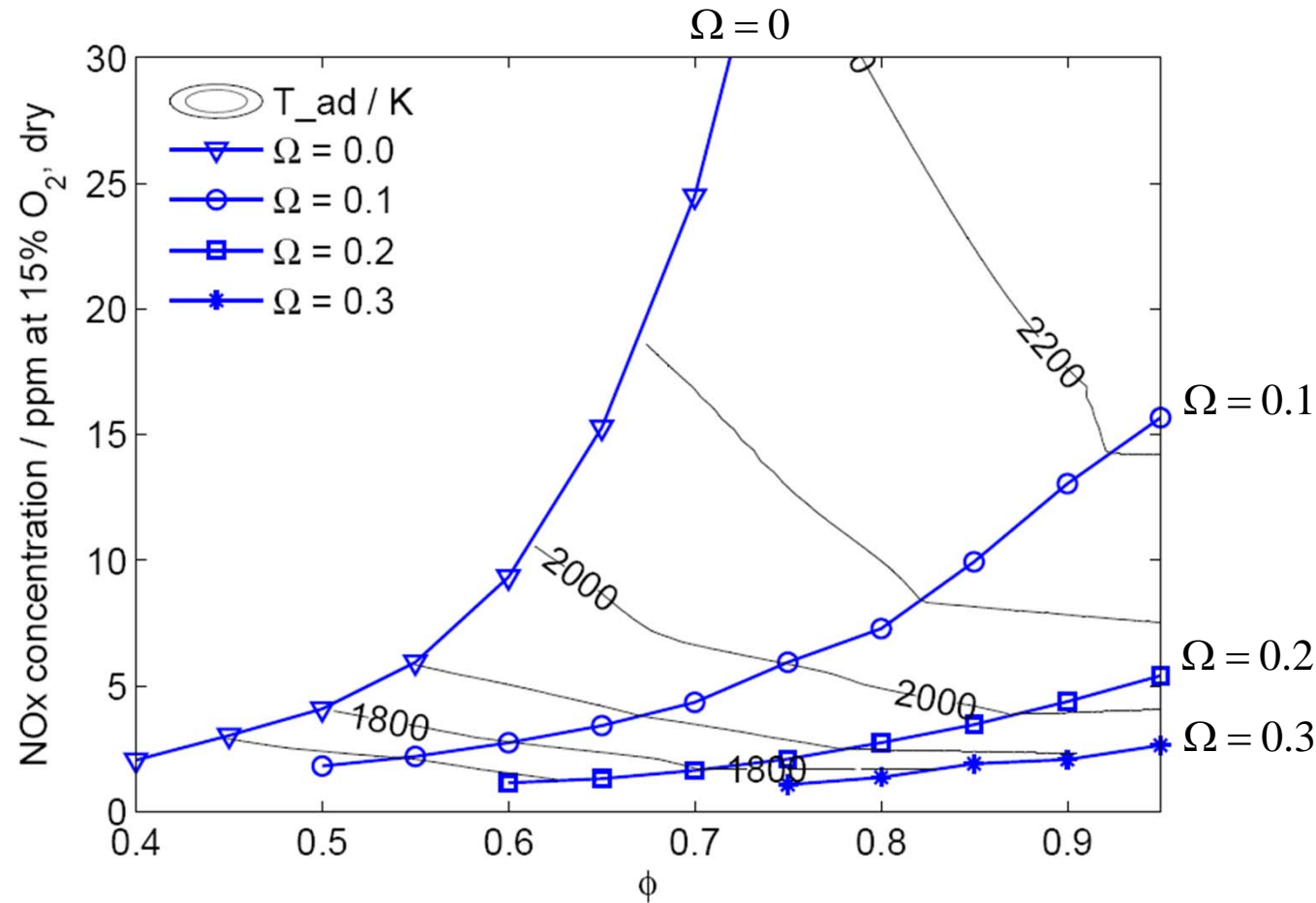
# OH Radical Concentration: Not significantly affected by steam



$T_{ad} = 1850 \text{ K}$

# NO<sub>x</sub> Emissions for Natural Gas:

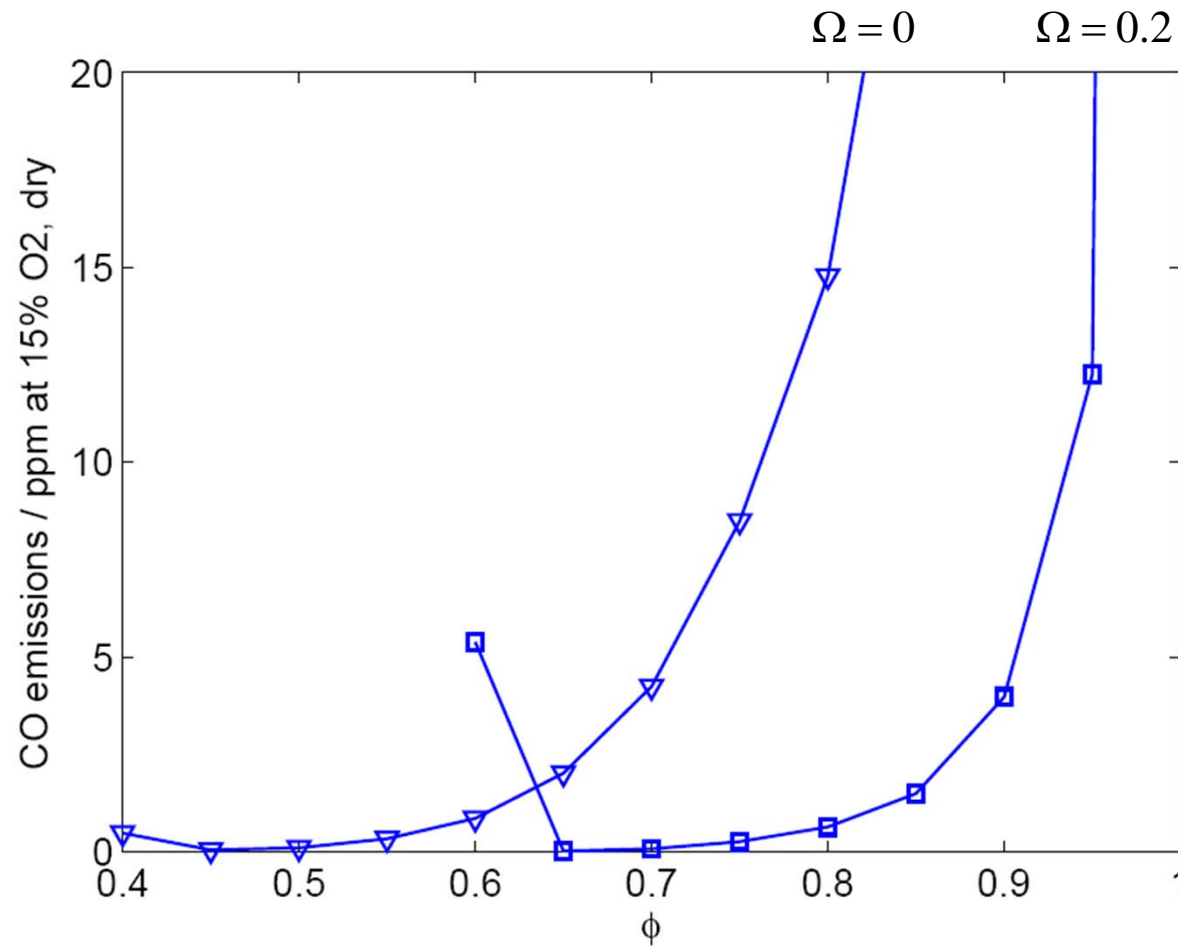
Steam reduces NO<sub>x</sub> even at same temperature



Measured NO<sub>x</sub>,  $T_{in} = 645$  K

# Measured CO Emissions:

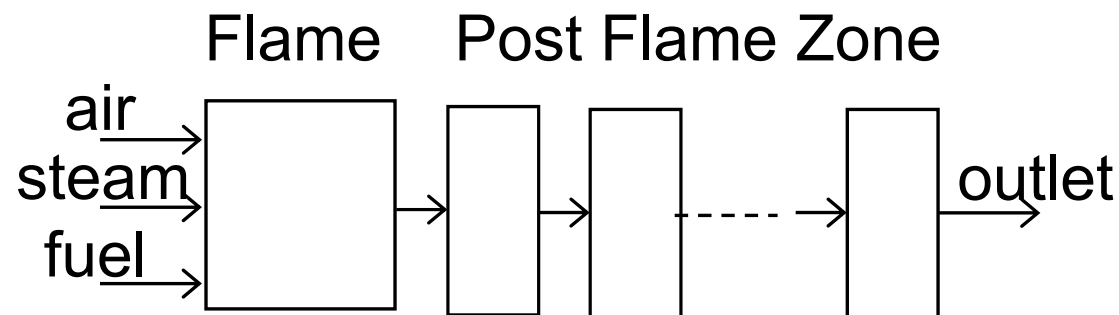
Steam does not noticeably affect CO



Measured CO,  $T_{in} = 645 \text{ K}$

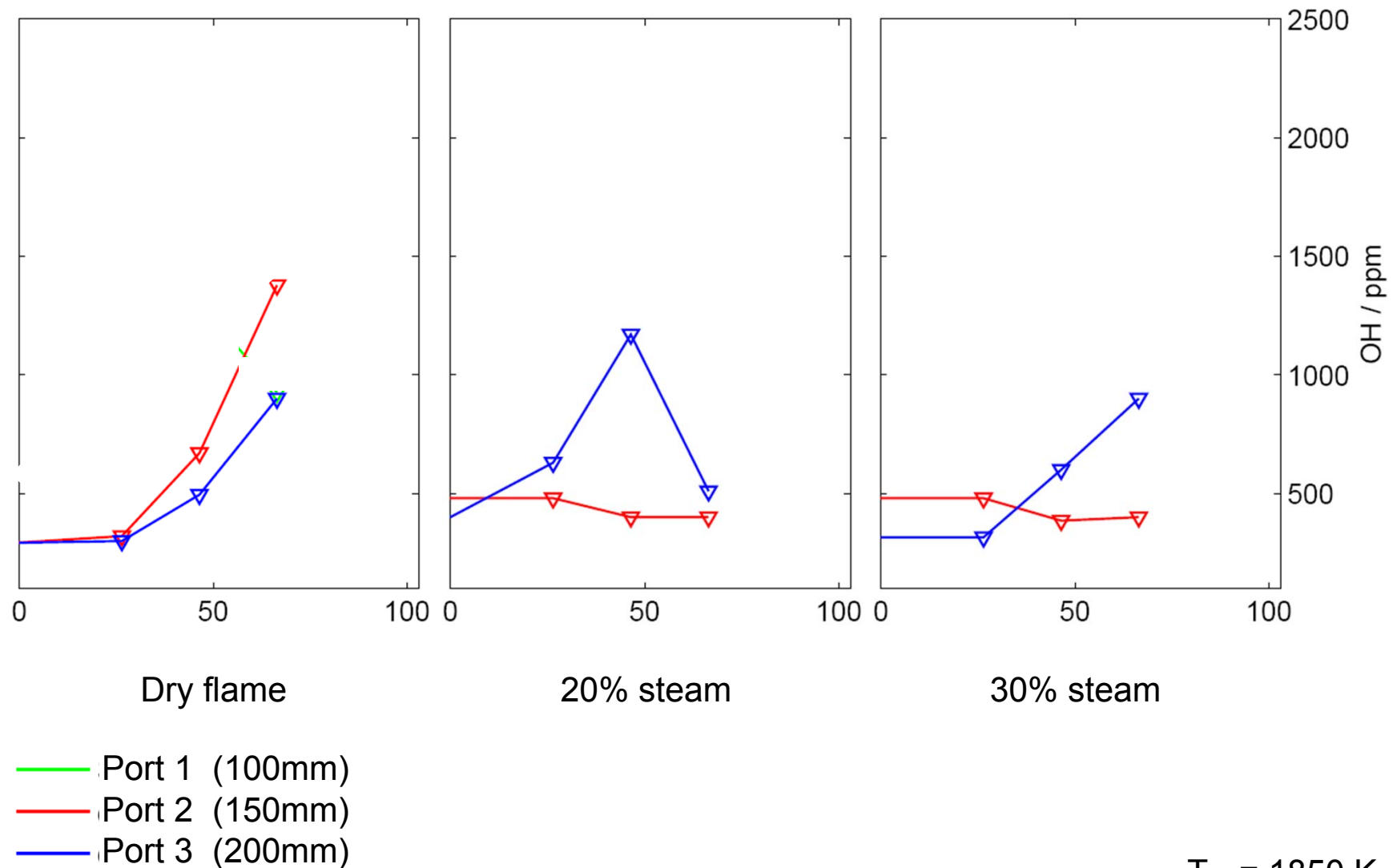
- Motivation and Background
- Experimental Setup and Results
- **Design of Reactor Network and Validation**
- Results of Network Model
- Conclusions

- Flame modeled by perfectly stirred reactor (PSR)
- Post flame zone modeled with a plug flow reactor (series of 20 PSRs)
- Heat loss:
  - Radiation (gray gas model and optical thin model)
  - Convective heat transfer based on measured cooling water temperature
- Reaction mechanisms:
  - GRI-Mech 3.0
  - Konnov “Reaction Mechanism for the Combustion of Small Hydrocarbons”, rev 05
- Investigated operating conditions:
  - Two different fuel concentrations:  $X_{\text{CH}_4} = 5.4\%$  and  $X_{\text{CH}_4} = 6.8\%$  ( $\Phi = 0.5 \dots 0.9$ )
  - Three flame temperatures:  $T_{\text{flame}} = 1670\text{K}, 1829\text{K}, 1970\text{K}$



# OH Radical Concentration:

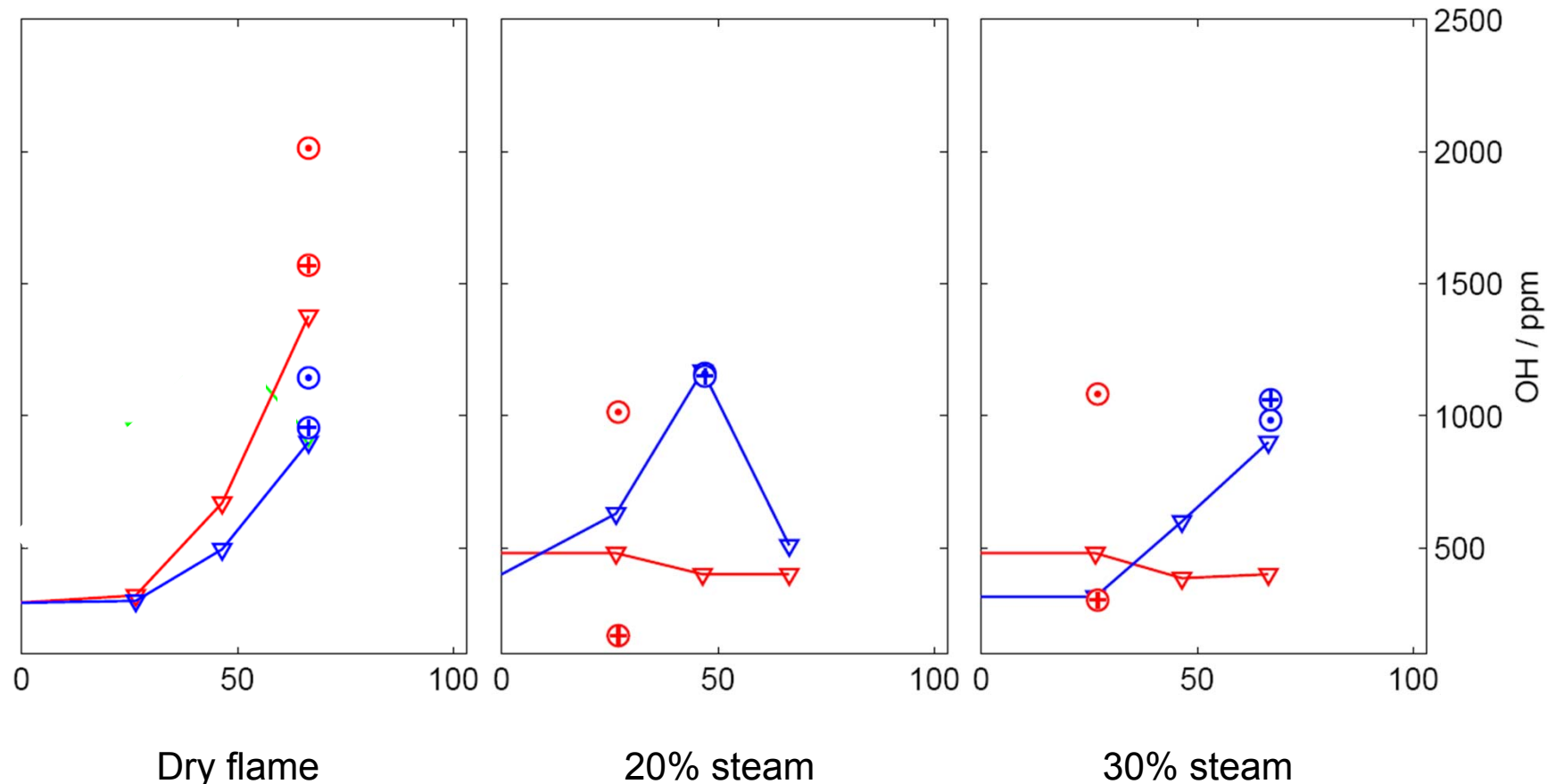
Not significantly affected by steam



$T_{ad} = 1850 \text{ K}$

# OH Radical Concentration:

Model predictions agree with experiments



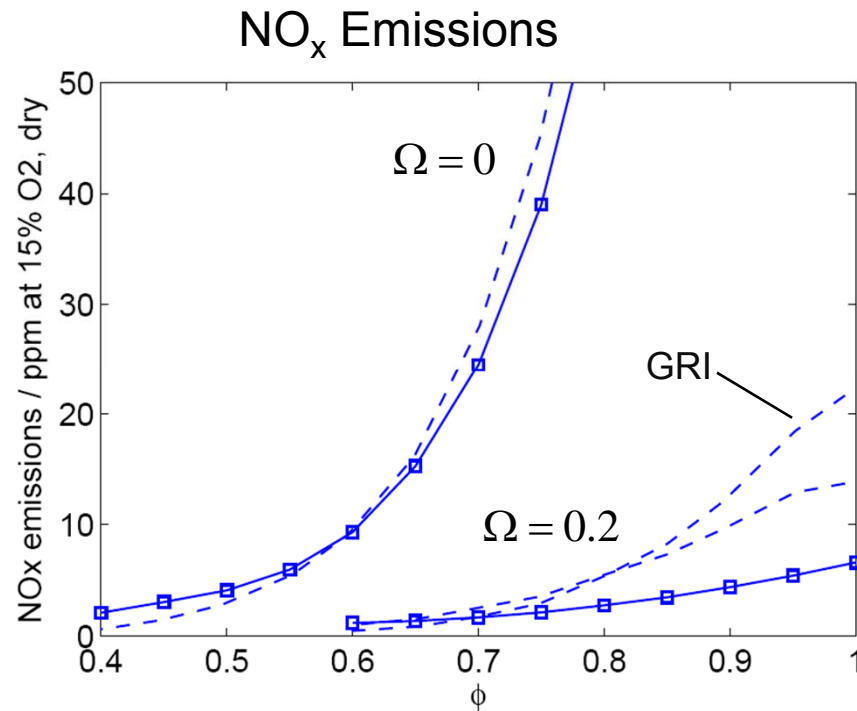
— Port 1 (100mm)  
 — Port 2 (Reactor 2) (150mm)  
 — Port 3 (Reactor 3) (200mm)

⊕ GRI-Mech 3.0  
 ⊕ Konnov reaction mechanism

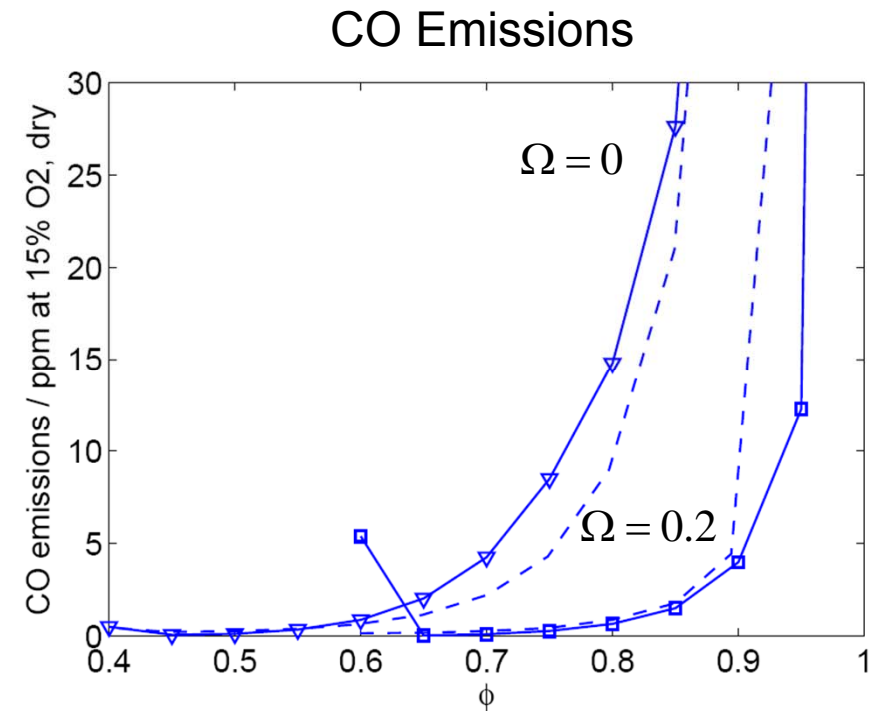
$T_{ad} = 1850 \text{ K}$

# Results of Network Model:

Trends of experimental results well predicted



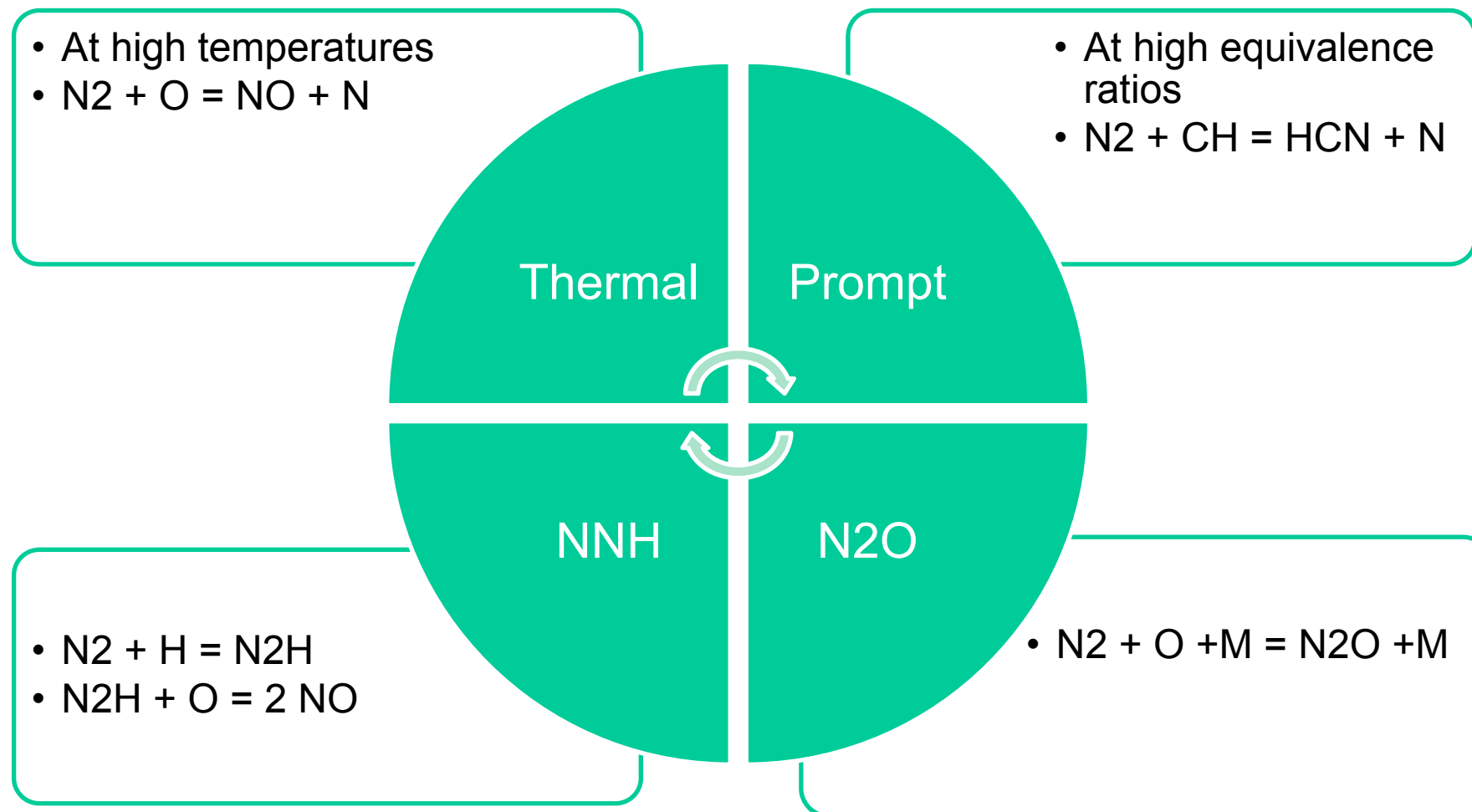
—■— Experimental    — Experimental  
- - - Simulation    - - - Simulation

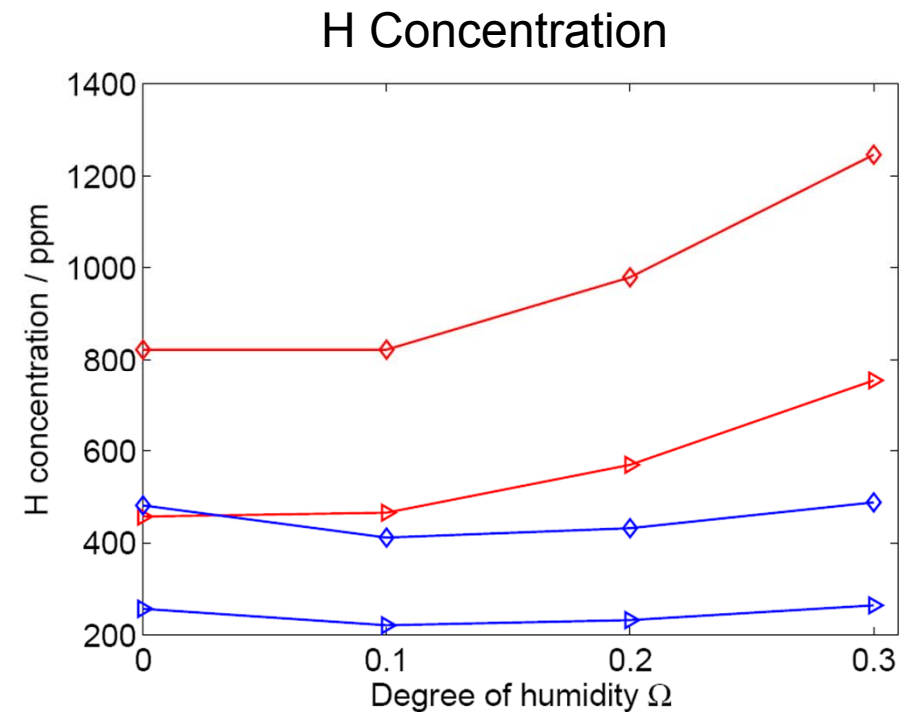
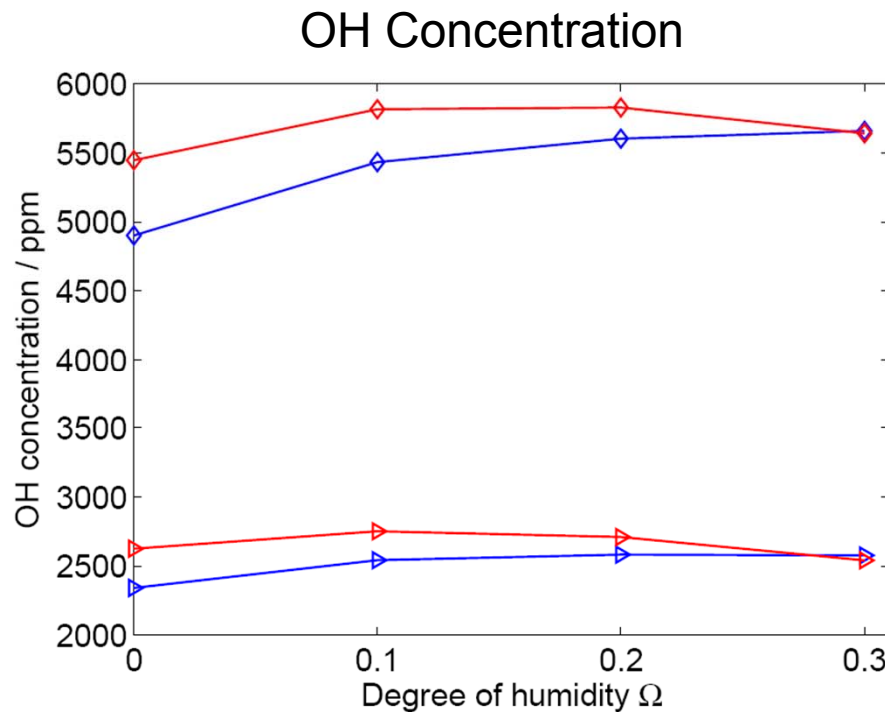


Measured and predicted emissions (Konnov)



- Motivation and Background
- Experimental Setup and Results
- Design of Reactor Network and Validation
- **Results of Network Model**
- Conclusions



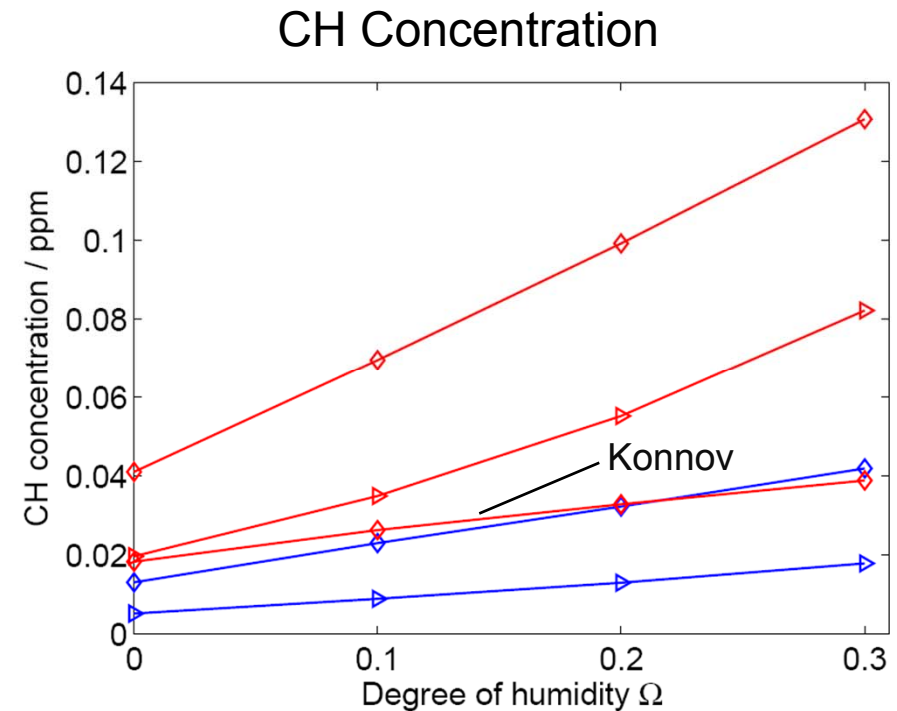
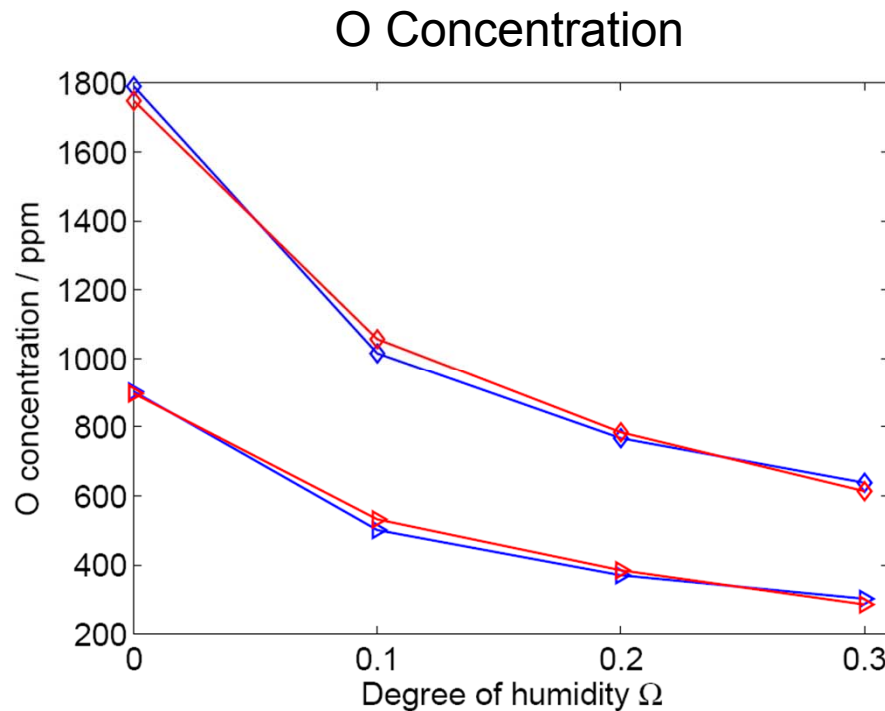


- CO formation  $CO + OH \rightarrow H + CO_2$  can be both increased and decreased at ultra-wet conditions
- $NO_x$  formation more affected by change in other species

- △—  $X_{CH_4} = 5.4\%$ ,  $T_{flame} = 1673K$
- △—  $X_{CH_4} = 6.8\%$ ,  $T_{flame} = 1673K$
- ◇—  $X_{CH_4} = 5.4\%$ ,  $T_{flame} = 1973K$
- ◇—  $X_{CH_4} = 6.8\%$ ,  $T_{flame} = 1973K$

Species concentrations in flame reactor (GRI)

# Results of Network Model: Prediction of very high CH concentrations

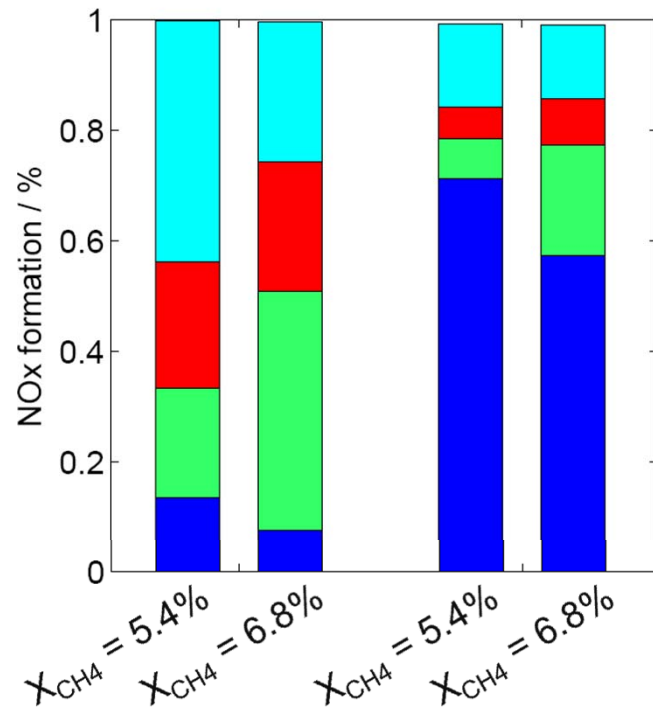


- Thermal, NNH, and N<sub>2</sub>O pathways restrained by reduced O concentration
- Prompt pathway increased due to higher CH concentration

$\blacktriangle$   $X_{CH_4} = 5.4\%, T_{flame} = 1673K$   
 $\blacktriangleright$   $X_{CH_4} = 6.8\%, T_{flame} = 1673K$   
 $\blacklozenge$   $X_{CH_4} = 5.4\%, T_{flame} = 1973K$   
 $\blacklozenge$   $X_{CH_4} = 6.8\%, T_{flame} = 1973K$

Species concentrations in flame reactor (GRI)

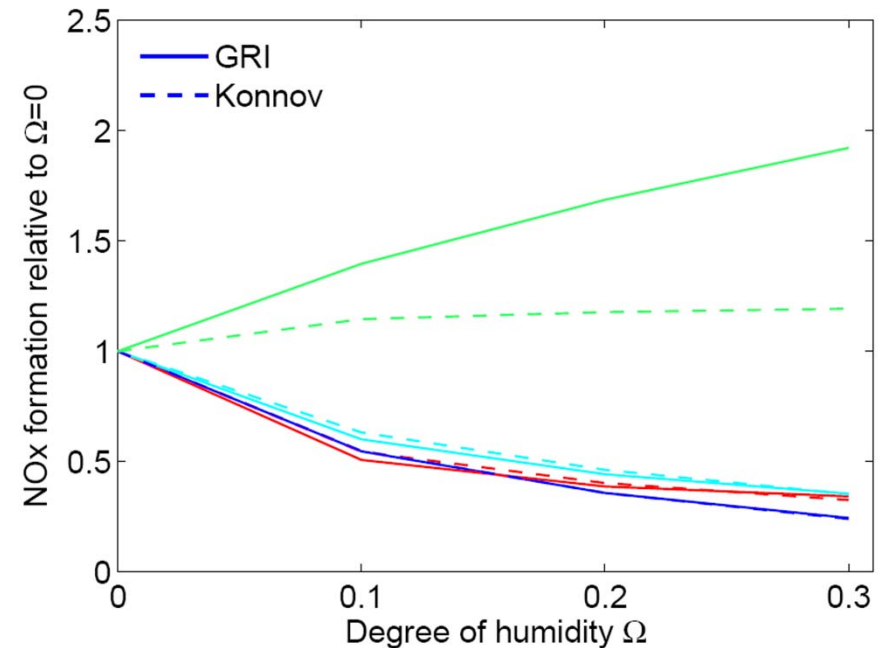
NO<sub>x</sub> pathways at dry conditions



$T_{\text{flame}} = 1670 \text{ K}$

$T_{\text{flame}} = 1970 \text{ K}$

NO<sub>x</sub> pathways at wet conditions



- GRI thermal
- GRI prompt
- GRI NNH
- GRI N2O

Calculated share of NO<sub>x</sub> formation pathways

## Experiments:

- Stable flame up to a degree of humidity of  $\Omega = 35\%$  for natural gas
- $\text{NO}_x$  emissions are significantly reduced
- CO is not noticeably affected by the steam (at atmospheric conditions)

## Investigation of chemistry:

- Developed model predicts the experimental results ( $\text{NO}_x$ , CO, OH) well
- Influence of steam depends strongly on the degree of dilution
- Thermal  $\text{NO}_x$  significantly reduced also at high temperatures
- Prompt  $\text{NO}_x$  formation is predicted to increase with steam content, and might be over-predicted by the reaction mechanisms

Thank you for your attention.